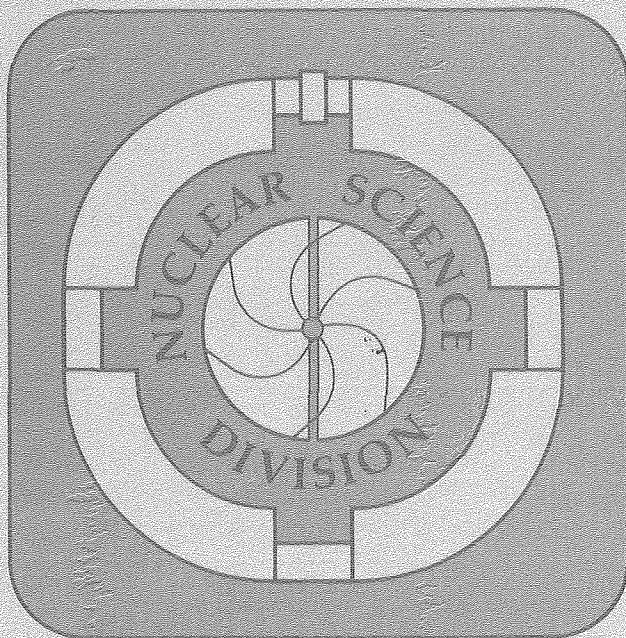# Lawrence Berkeley Laboratory
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APPLICATION OF THE IMAGINARY TIME STEP METHOD TO
THE SOLUTION OF THE STATIC HARTREE-FOCK PROBLEM

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DISCLAIMER

APPLICATION OF THE IMAGINARY TIME STEP METHOD TO THE SOLUTION OF THE STATIC HARTREE-FOCK PROBLEM

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ABSTRACT

A method of solution of the static Hartree-Fock problem is proposed. The method, based upon the extension of the method of solution of the time-dependent Hartree-Fock problem to imaginary time, promises to be more efficient, and applicable to more complex systems than previously proposed numerical methods.

I. INTRODUCTION

The mathematical question of the existence of a solution to a system of coupled nonlinear equations, such as that which occurs in the Hartree-Fock (HF) approximation, is still unanswered. On the other hand, several practical methods have been proposed, which solve the problem numerically. These methods rely on iterative procedures, which are pursued until an ad hoc defined stability of the results is achieved from one iteration to the next. Contrary to the situation found in solving most sets of nonlinear equations, the solution of the HF equations is subject to a stringent numerical check, which guarantees that the solution of the iterative procedure is indeed a solution of the HF equations. Before describing this check, which depends upon the self-consistency of the HF approximation, we shall first present briefly the currently most popular method for solving the equations. This method can be analyzed in terms of four distinct steps, the last two of which are iterated.

Step 1: Select a convenient parameterization of the single particle orbitals, whose determinant represents the variational wave function. This can be accomplished either by expanding the wave functions in a basis,[1] in which case the expansion coefficients are to be determined, or by discretizing the wave functions on a spatial mesh, in which case the values of the wave functions at the mesh points are to be determined.[2]

Step 2: Select a physically reasonable approximation (e.g., Wood-Saxon or oscillator potential) to the one-body hamiltonian, $h^{(0)}$, where the iteration number is denoted by a superscript.

Step 3: Compute the matrix elements of the one-body hamiltonian $h^{(n)}$ in the variational space selected in step 1, and determine the lowest eigenstates of $h^{(n)}$ in this space. This is generally[3] achieved by diagonalizing $h^{(n)}$ to obtain simultaneously the single particle wave functions $\{\psi_i^{(n)}\}$, and corresponding energies $\{\varepsilon_i^{(n)}\}$, where the subscript, i, labels the orbitals. At this stage the HF approximation, $E^{(n)}$, to the total energy E may also be computed.

Step 4: Construct $h^{(n+1)}$ by taking the matrix elements of the effective many body interaction $\hat{v}$ with respect to the wave function formed by occupying the orbitals of lowest energy determined in step 3.

Steps 3 and 4 are then iterated until stability is achieved. For example, the iteration may be terminated when either the $\{\varepsilon_i^{(n)}\}$ or $E^{(n)}$ differs from the $\{\varepsilon_i^{(n-1)}\}$ or $E^{(n-1)}$, respectively, by less than a predetermined amount.

The stringent check on the iterated solution, which was referred to above, is provided by the equality of the calculation of

$$E = \frac{1}{2} (T + \sum_{1}^{A} \varepsilon_i) \qquad (1.1)$$

or as

$$E = T + \langle v \rangle$$

where $\langle \hat{v} \rangle$ is the expectation value of the effective potential $\hat{v}$ and T the expectation value of the kinetic energy

$$T = \frac{\hbar^2}{2m} \sum_{i=1}^{A} \int |\nabla \psi_i|^2 \, d^3r \; . \qquad (1.2)$$

Equation (1.1) is satisfied only when self-consistency is achieved between the eigenfunctions, $\{\psi_i\}$, of h, and the hamiltonian h, which is itself a function of the eigenfunctions. The criterion that Eq. (1.1) be satisfied represents a critical test of the numerical method employed to solve the equations. It would, for example, reveal the existence of coding errors, which nevertheless maintain the convergence properties of the iterative procedure but is more usefully employed as a convergence criterion.

The critical computational procedure in the solution arises at step 3. Indeed, the diagonalization of the hamiltonian matrix can only be performed conveniently for small variational spaces. For studies of medium mass nuclei, this can be easily achieved by the use of an oscillator basis. However for heavy deformed nuclei, such as the actinides, it is necessary to include up to 14 oscillator shells in the basis, in order to calculate the total energy within an accuracy of about 10 MeV.[4] In these cases non-sparse matrices of the order of 100x100 must be handled. Moreover, since the basis must necessarily be truncated, the effects on the solution of changes in the parameters

of the basis, such as the oscillator frequency, and the deformation

parameters must be studied, and optimal values of the parameters

chosen. Further, for very exotic shapes, such as those occurring in

the collision of ions or or in that part of the fission path between

saddle point and scission point, a usable oscillator basis is no

longer adequate. In such cases, two-center bases can be employed.

However their use introduces an additional parameter in the definition

of the basis and makes the optimization process yet more cumbersome.

Finally, we note that the description of triaxial medium or heavy mass

nuclei would require huge bases dependent upon at least three param-

eters, and that an accurate solution of the HF equations in such a

basis appears to be hopeless.

The natural way to avoid the basis generated problems outlined

above is to discretize the wave functions on a three-dimensional

spatial mesh. Firstly, such a parameterization is not likely to

influence the shape of the wave function, as could a particular choice

of oscillator basis. Secondly, such a parametrization depends upon but

a single quantity, the size, Δx, of the mesh.[5] Moreover, in contrast

to the optimization of the oscillator parameters, which requires a

quasi-random search, it is evident that the smaller Δx, the more

accurate the calculation. In practice a mesh size of the order of

1 fm insures sufficient accuracy. This may be seen by examining

Table 1, in which the kinetic and total energies of the nuclei ^{16}O

and ^{40}Ca are compared as calculated using a 1.0 fm mesh, an 0.8 fm

mesh, and analytically.

Even with such reasonably large values of Δx, the number of mesh

points required in order to obtain a satisfactory description of a

nucleus, and particularly of its surface, varies between several

hundred in the case of two dimensional, axially symmetric systems,

and several thousand in the case of three dimensional systems. Clearly,

the repeated diagonalization of the large matrices generated in such

problems becomes intractable. In addition the diagonalization proce-

dure provides unuseful information on highly excited levels which

influence neither the HF hamiltonian nor the ground state energy. It

is therefore our purpose in this paper to present an alternative method

of solving the HF equations which requires that one deals only with

occupied single particle levels, and is particularly adaptable for

use with local or quasi-local HF hamiltonians, as occur when some of

the most widely used effective interactions, such as that of Skyrme[3]

are employed. Indeed, with such interactions, the coordinate space

representation of the single particle hamiltonian takes the form

$$h(\underset{\sim}{r}) = -\underset{\sim}{\nabla} \cdot \frac{\hbar^2}{2m^*(\underset{\sim}{r})} \underset{\sim}{\nabla} + V(\underset{\sim}{r}) \qquad (1.3)$$

in which $m^*(\underset{\sim}{r})$ and $V(\underset{\sim}{r})$ are respectively the effective mass and the

self-consistent potential. When discretized on a spatial mesh, h

becomes a sparse matrix with non-zero matrix elements only near the

diagonal. Much less storage space is required to handle such a matrix,

and the problem thus becomes tractable with standard computing

facilities.

The imaginary time step method, as we choose to refer to it, is so simple that it is difficult to imagine that we have been the first to discover its application to non-linear problems. Nevertheless, we feel justified in coining a name for it, first, because we were unable to find earlier references to the method in the domain of non-linear equations, and second, because we have been the first to employ the method in the solution of the nuclear HF problem. What follows is neither a rigorous mathematical justification of the method, nor a general numerical analysis. Rather we shall mainly describe the method in such a manner as to emphasize its physical justifications. We shall also prove, in the following section, that in the limit of an infinitesimal time step, the iterated approximation converges to the HF solution, and provides at the same time, the eigenstates of the one body hamiltonian. In section 3 we shall illustrate some numerical aspects of the method with typical solutions for nuclear systems.

II. PRINCIPLE OF THE IMAGINARY TIME STEP METHOD

The name is derived from the analogy of the method with that employed to solve the time-dependent Hartree-Fock (TDHF) equations

$$i\hbar \frac{\partial \psi_j}{\partial t} = h(t)\psi_j(t) \qquad j = 1,\ldots,A \qquad (2.1)$$

Equations (2.1) represent a set of A coupled, nonlinear, partial differential equations, in which the spatial derivatives are due to the kinetic energy term $-\hbar^2/2 \; \underset{\sim}{\nabla} \cdot \frac{1}{m^*} \underset{\sim}{\nabla}$ of h. By discretizing in time, and introducing a time step Δt, with $t_n = n\Delta t$, the solution, $\{\psi_j^{(n+1)}\}$, of the partial differential equations at time t_{n+1} may be approximated in terms of the solution at time t_n by

$$|\psi_j^{(n+1)}\rangle = \exp(-\frac{i}{\hbar} \Delta t \; h^{(n+\frac{1}{2})}) |\psi_j^{(n)}\rangle \qquad j = 1,\ldots,A \qquad (2.2)$$

in which $h^{(n+\frac{1}{2})}$ denotes the numerical approximation to the hamiltonian $h(t)$ at time $(n+\frac{1}{2})\Delta t$. Various methods of calculating $h^{(n+1/2)}$ are discussed in references 6-8. Two properties of the exponential operator of Eq. (2.2) should be mentioned here. The first property is its unitarity, which ensures that the orthonormality of the initial set of wave functions will be preserved in the time evolution. The second property, crucial for the TDHF problem, deals with the conservation of energy. In appendix B of reference g, it is shown that for any two orthonormal sets of wave functions $\{\psi_j^{(n+1)}\}$ and $\{\psi_j^{(n)}\}$ the difference of the HF energies can be written as[10]

$$E^{(n+1)} - E^{(n)} = \sum_{j=1}^{A} \int d^3r (\psi_j^{(n+1)*} h^{(n+\frac{1}{2})} \psi_j^{(n+1)} - \psi_j^{(n)*} h^{(n+\frac{1}{2})} \psi_j^{(n)})$$

$$(2.3)$$

By introducing the density matrix, $\rho^{(n)}$, which, in the coordinate representation may be written as

$$\langle \underset{\sim}{r} | \rho^{(n)} | \underset{\sim}{r}' \rangle = \sum_{j=1}^{A} \langle \underset{\sim}{r} | \psi_j^{(n)} \rangle \langle \psi_j^{(n)} | \underset{\sim}{r}' \rangle$$

$$= \sum_{j=1}^{A} \psi_j^{(n)} (\underset{\sim}{r}) \psi_j^{(n)*} (\underset{\sim}{r}')$$

$$(2.4)$$

Eq. (2.3) takes the simpler form

$$E^{(n+1)} - E^{(n)} = Tr(h^{(n+\frac{1}{2})} (\rho^{(n+1)} - \rho^{(n)})) \, .$$

$$(2.5)$$

If the wave functions are evolved according to Eq. (2.2), the density matrix at time $(n+1)\Delta t$ is then given in terms of the matrix at time $n\Delta t$ by

$$\rho^{(n+1)} = \exp(-\frac{i}{\hbar} \Delta t \, h^{(n+\frac{1}{2})}) \, \rho^{(n)} \, \exp(\frac{i}{\hbar} \Delta t \, h^{(n+\frac{1}{2})}) \, .$$

$$(2.6)$$

It then follows, from Eq. (2.5), and the cyclic invariance of the trace, that $E^{(n+1)} - E^{(n)} = 0$. The approximation method thus conserves the HF energy. Given this property, it is natural to hypothesize that the replacement of the time step Δt by the imaginary quantity $-i\Delta t$ will lead to a decrease of the HF energy. This is precisely what we shall now demonstrate, at least to first order in Δt. Accordingly, we

introduce the positive parameter $\lambda = \Delta t / \hbar$, and study the transformation

$$|\Psi_j^{(n+1)}\rangle = \exp(-\lambda h^{(n+\frac{1}{2})})|\psi_j^{(n)}\rangle \qquad j = 1,\ldots,A \qquad (2.7)$$

Note that in the above formula, we have introduced a different symbol, capital psi, for the wave functions generated by the transformation. The functions $\{\Psi_j\}$ differ from the $\{\psi_j\}$ of the TDHF iteration in that they do not constitute an orthonormal set. They must therefore be orthonormalized before proceeding to the next iteration. The imaginary time step method can thus be described as follows:

Step 1: Select an initial set of single particle wave functions, $\{\psi_j^{(0)}\}$. For example one could work with the values of harmonic oscillator or Nilsson wavefunctions on an appropriately discretized coordinate mesh.

Step 2: Construct from the wave functions the hamiltonian $h^{(n)}$ (which, in the HF approximation is a function of $\langle \underset{\sim}{r}|\rho^{(n)}|\underset{\sim}{r}'\rangle$).

Step 3: Generate the set of wave functions $\{\Psi_j^{(n+1)}\}$, via the transformation given in Eq. (2.7).

Step 4: Orthonormalize the $\{\Psi_j^{(n+1)}\}$ to obtain the $\{\psi_j^{(n+1)}\}$.

Steps 2, 3, and 4 are then iterated until convergence is attained. The major difference with the numerical procedure used to solve the TDHF equations is the orthogonalization of the wave functions performed in step 4. Although the method of orthogonalization is arbitrary, in practice we employ the Schmidt method, because the wave functions ψ_j

then converge to the eigenfunctions of the HF hamiltonian. An alternate method of orthogonalization would result in wavefunctions which differ from the ψ_j by a unitary transformation, and hence lead to the same density matrix.

Rather than discussing the manner in which the exponential transformation, Eq. (2.7), is actually performed, we shall postpone this discussion to section 3, and shall now analyze some general properties of the iterative scheme.

We begin by showing that the imaginary time step method leads to the eigenstates of the hamiltonian h. For this purpose, the self-consistency condition is not important, and the dependence of h upon the iteration number need not be considered. Denote by $\{\phi_j\}$, $j = 1,\ldots,\infty$ the eigenstates of h, ordered with respect to increasing single particle energies ε_j. At a given time step n, the A wave functions $\psi_j^{(n)}$ may be expanded in the basis $\{\phi_j\}$,

$$|\psi_j^{(n)}\rangle = \sum_{k=1}^{\infty} c_{jk} |\phi_k\rangle \quad , \tag{2.8}$$

so that

$$|\psi_j^{(n+1)}\rangle = \sum_{k=1}^{\infty} c_{jk} \exp(-\lambda e_k) |\phi_k\rangle \quad . \tag{2.9}$$

It is clear from Eq. (2.9) that only the lowest eigenstate is retained after several exponential transformations. If a Schmidt orthogonalization is then performed, the jth wave function will converge toward

ϕ_j^*. Parenthetically we note that it is of no use to add to the hamiltonian a negative constant $-h_0$ in order to hasten the convergence. Indeed, since this constant will enhance each component by precisely the same factor $e^{\lambda h}0$, its effect will be totally eliminated in the Schmidt orthonormalization.

Having shown that the method yields the lowest eigenstates of h, we now show, to first order in λ, that $h^{(n)}$ converges toward the self-consistent hamiltonian. In the limit of small λ, Eq. (2.7) may be approximated as

$$|\psi_j^{(n+1)}\rangle = (1-\lambda h^{(n+\frac{1}{2})})|\psi_j^{(n)}\rangle + O(\lambda^2) \ .$$

Upon Schmidt orthogonalization, we obtain[11] the wave functions

$$|\psi_j^{(n+1)}\rangle = (1+\lambda(\varepsilon_{jj}^{(n)}-h^{(n+\frac{1}{2})}))|\psi_j^{(n)}\rangle + 2\lambda \sum_{k=1}^{j-1} \varepsilon_{kj}^{(n)}|\psi_k^{(n)}\rangle \quad (2.10)$$

$$+ O(\lambda^2) \ ,$$

where

$$\varepsilon_{kj}^{(n)} = \langle \psi_k^{(n)}|h^{(n+\frac{1}{2})}|\psi_j^{(n)}\rangle \ . \tag{2.11}$$

We next construct the change in the one body density

$$\rho^{(n+1)}-\rho^{(n)} = \sum_{j=1}^{A} |\psi_j^{(n+1)}\rangle \langle \psi_j^{(n+1)}|-|\psi_j^{(n)}\rangle \langle \psi_j^{(n)}| \ . \tag{2.12}$$

Substituting for $\psi_j^{(n+1)}$ according to Eq. (2.10), we obtain (to first order in λ) the result

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*The validity of the statement is clear if one recalls that the Schmidt procedure ensures the orthogonality of the jth state to the previously orthogonalized states 1, 2...j-1.

$$\rho^{(n+1)} - \rho^{(n)} = -\lambda(\rho^{(n)} h^{(n+\frac{1}{2})}(1-\rho^{(n)}) + (1-\rho^{(n)}) h^{(n+\frac{1}{2})}\rho^{(n)}) . \quad (2.13)$$

The change in the HF energy may now be found by substituting Eq. (2.13) in Eq. (2.5). Using the cyclic invariance of the trance, we have

$$E^{(n+1)} - E^{(n)} = -\lambda \text{Tr}(h^{(n+\frac{1}{2})}(\rho^{(n)} h^{(n+\frac{1}{2})}(1-\rho^{(n)}) + (1-\rho^{(n)}) h^{(n+\frac{1}{2})}\rho^{(n)}))$$

$$= -2\lambda \text{Tr}(\rho^{(n)} h^{(n+\frac{1}{2})}(1-\rho^{(n)}) h^{(n+\frac{1}{2})}) .$$

Consider now the operator

$$A^\dagger = \rho^{(n)} h^{(n+\frac{1}{2})}(1-\rho^{(n)}) . \quad (2.14)$$

Using the cyclic invariance of the trace, the idempotency of the density matrix ($\rho^2 = \rho$), and the hermiticity of ρ and h, we have

$$\text{Tr}(A^\dagger A) = \text{Tr}(\rho^{(n)} h^{(n+\frac{1}{2})}(1-\rho^{(n)})(1-\rho^{(n)}) h^{(n+\frac{1}{2})}\rho^{(n)})$$

$$= \text{Tr}(\rho^{(n)} h^{(n+\frac{1}{2})}(1-\rho^{(n)}) h^{(n+\frac{1}{2})}) .$$

We have thus succeeded in showing that

$$E^{(n+1)} - E^{(n)} = -2\lambda \text{Tr}(A^\dagger A) + O(\lambda^2) , \quad (2.15)$$

from which we conclude that the energy must decrease from iteration n to iteration n+1, until the operator A becomes equal to zero. Since the latter condition may be formulated as

$$[h^{(n+\frac{1}{2})}, \rho^{(n)}]\rho^{(n)} = 0 , \quad (2.16)$$

it is equivalent[12] to the HF condition $[h,\rho] = 0$. We have consequently

shown that for values of λ sufficiently small to justify the linear

expansion, the imaginary time step method results in a monotonic

decrease in the HF energy, from iteration to iteration, until the

density converges to the HF density. We have additionally shown that

if Schmidt orthogonalization is performed after each iteration, as

detailed by Eq. (2.10), the wave functions ψ_j converge to the lowest

eigenstates of h. The diagonal elements of the matrix ε_{kj} correspond-

ingly converge to the eigenvalues of h.

The imaginary time step method may be related to another, re-

cently proposed method[13] for solving the static HF equations by

considering the transformation

$$|\psi_j^{(n+1)}\rangle = (1-\lambda h^{(n+\frac{1}{2})})|\psi_j^{(n)}\rangle + \lambda \sum_{k=1}^{A} \varepsilon_{kj}^{(n)}|\psi_k^{(n)}\rangle + 0(\lambda^2). \quad (2.17)$$

Equation (2.17) represents a more symmetric orthogonalization of the

Ψ_j's generated by the transformation of Eq. (2.7) than that accomplished

by the Schmidt method. The Eq. (2.17) differs from Eq. (2.10) in

that all of the occupied states contribute to the sum, each weighted

by the factor $\lambda\varepsilon_{kj}$, in Eq. (2.17), whereas only the states $k < j$, each

weighted by the factor $2\lambda\varepsilon_{kj}$, contribute to the sum in Eq. (2.10).

It is easily verified that Eq. (2.13) remains unchanged if the

transformation Eq. (2.17) is employed rather than Eq. (2.10). Our

discussion concerning the convergence of ρ to the HF solution therefore

remains valid. As previously noted, however, the ψ_j's and ε_{jj}'s will

not be the eigenstates and eigenvalues, respectively, of h. In order

to facilitate comparison with the method of Di Toro et al[13], we use the property

$$\rho^{(n)} | \psi_j^{(n)} \rangle = | \psi_j^{(n)} \rangle \qquad j = 1, \ldots, A$$

to rewrite Eq. (2.17) as

$$| \psi_j^{(n+1)} \rangle = (1 + \lambda [\rho^{(n)}, h^{(n+\frac{1}{2})}]) | \psi_j^{(n)} \rangle + O(\lambda^2). \quad (2.18)$$

The unitarity of the transformation is then obvious, and a natural generalization of Eq. (2.18) is

$$| \psi_j^{(n+1)} \rangle = \exp(\lambda [\rho^{(n)}, h^{(n+\frac{1}{2})}]) | \psi_j^{(n)} \rangle . \qquad (2.19)$$

Di Toro et al[13] have investigated the above transformation, and have further proposed a procedure for determining an optimal value of λ for each iteration. However from our point of view, this method, as described in Ref. 13, suffers from the fact that it explicitly deals with the density and hamiltonian matrices, so that its use has up to now been restricted to HF calculations where the standard method discussed in the introduction has already been proven valid. Of course when the matrices ρ and h are unmanageably large, the transformation of Eq. (2.19) can still be implemented. However the computation would proceed more slowly than the imaginary time step method (2.7). In this connection one should note that although the transformation given by Eq. (2.19) is unitary, the calculational necessity of truncating the exponential expansion would destroy exact unitarity, and

reorthonormalization of the wave functions would still be necessary.

In concluding this section, we point out a practical simplification of the algorithm used in the imaginary time step method, as compared to that required in TDHF. As is easily deduced, from the linear dependence of h upon ρ, and the fact that $\rho^{(n+1)} - \rho^{(n)}$ is of first order in λ, Eqs. (2.10)-(2.15) retain their validity when $h^{(n+1/2)}$ is replaced by $h^{(n)}$. Indeed, we have found in practice that the algorithm remains stable, and the iterated equations converge to the HF solution, when this time saving replacement is made.

III. APPLICATION OF THE IMAGINARY TIME STEP METHOD

In the last years, the imaginary time step method has been used to study a number of physical problems. For example, the method has been employed to calculate the ground states of projectile and target nuclei, to be used as the initial wave functions in TDHF calculations,[14] and to obtain deformation energy curves, via constrained HF calculations, for studying the collision of various 1p and 2s-1d shell nuclei.[15] With slight modification, the method has also been used to compute mass parameters pertinent to the reactions $^{12}C + ^{12}C$ and $^{16}O + ^{16}O$.[16] In this section, we shall focus only on some practical aspects of the calculations. In particular, we shall study the influence of the magnitude of the parameter λ, and of the number of terms retained in the exponential in Eq. (2.7), in calculations of the ground state of ^{40}Ca.

The code employed to perform the calculations allows triaxial deformation. The sole spatial symmetries imposed are planar symmetry with respect to the y=0 plane and the z=0 plane, so that the code can be used to study left-right assymetric nuclear systems. The single particle wave functions are discretized on a regular, three dimensional cartesian grid. In the calculations to be discussed below, the mesh size is equal to 1 fm, and the number of mesh points in the x, y, and z directions is 15, 7, and 7, respectively, thereby yielding a variational space of dimensionality 735. Before analyzing the factors which govern the convergence of the solutions, we first discuss our criteria for terminating the iterations. As previously discussed,

there exist two distinct convergence criteria, which, in principle,
can be satisfied separately. First, the Slater determinant is to
converge to the HF solution, and the energy concurrently to decrease
to a minimum. An excellent check that this is achieved is provided
by the test mentioned in the introduction. Second, the single particle
wave functions are to converge to the eigenstates of h. As the satis-
faction of the latter condition guarantees the former, while the
converse is not true, we have adopted the second criterion as the
basis for terminating the calculations. To be specific, we have
chosen, as a convenient measure of the quality of the eigenstates,
the mean square deviation of the single particle energies,

$$\Delta h = \sum_j \left(\langle \psi_j | h^2 | \psi_j \rangle - \langle \psi_j | h | \psi_j \rangle^2 \right)^{1/2} .$$

Typically, we require Δh to be less than 1 MeV, which yields an
accuracy of roughly 1% or better for the eigenvalues of the occupied
states.[17] Since the loss of precision in the numerical results due
to the finite mesh size exceeds by several orders of magnitude that
due to the imaginary time step algorithm, we shall not compare the
results with "exact" results. Such a comparison can be found in the
appendices of Ref. 9, and in Ref. 18.

We now turn to the question of the influence of the parameter λ.
As previously noted, the exponential time evolution operator must
necessarily be approximated by a truncated expansion. In this analysis
of the influence of λ we use a five term approximation to the
exponential. The results are displayed in Fig. 1, in which the

difference between the nth approximation to the HF energy and the HF energy is plotted as a function of $t^{(n)} = n\Delta t$, for several values of $\Delta t = \lambda \hbar$. The initial wave function of the ^{40}Ca nucleus is a determinant of harmonic oscillator functions. As may be seen from the figure, for values of Δt less than or equal to 0.04×10^{-22}s, the calculation converges. In fact, further decrease of Δt not only causes no particular improvement, but instead only increases the computation time, since more iterations are required to arrive at a given total time, t.

The influence of the number of terms in the expansion of the exponential operator is illustrated in Fig. 2. In this figure, the difference between the nth approximation to the HF energy and the HF energy is plotted as a function of $t^{(n)}$ for expansions of the operator consisting of 2,3, . . . , and 10 terms. In all cases, the time step $\Delta t = 0.08 \times 10^{-22}$s. As may be seen from the figure, the method converges, for all practical purposes, when at least eight terms are retained in the approximation to the exponential for this particular time step. In fact, based upon experience, we have come to the conclusion that arbitrarily precise numerical results can be obtained with any value of Δt, provided a sufficient number of terms is retained in the exponential expansion. In general, we have found that computational efficiency is improved by using a small enough time step so that a four or five term expansion is sufficient. For this purpose, the value $\Delta t \simeq 0.04 \times 10^{-22}$s is suitable when the mesh size $\Delta x = 1$ fm is used.

IV. CONCLUSION

We have introduced a new method for solving the Hartree-Fock equations, that is specifically applicable to large systems. In addition to being applicable to problems for which most previous methods are unfeasible it is also computationally more efficient than alternate schemes. While our utilization has been restricted to the nuclear Hartree-Fock problem we believe this procedure may be of value to a much wider class of non-linear problems

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Table 1. Comparison of the kinetic energy T and H.F. energy E cal-
culated from discretized oscillator wave functions with the
analytical values. The oscillator parameters $\sqrt{m\omega/\hbar}$ are
.275 fm^{-2} for ^{16}O and 0.25 fm^{-2} for ^{40}Ca. The spatial
derivatives occurring in the calculation of the kinetic
energy are calculated with a 9-point method and that occurring
in the rest of the H.F. energy with a 5-point method. The
interaction used to calculate the H.F. energy is the Skyrme
force SIII as described in Ref. 3. The mesh size Δx is given
in fm and the energies in MeV.

	^{16}O		^{40}Ca	
	T	E	T	E
$\Delta x = 0.8$	205.280	-102.803	622.006	-307.308
$\Delta x = 1$	205.253	-102.901	621.933	-307.656
analy	205.288	-102.801	622.086	-306.730

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10. As is shown in Ref. 9, when to body forces only are present, $h^{(n+1/2)} = \frac{1}{2} (h^{(nth)} + h^{(n)})$ is required in order to derive Eq. (2.3).

11. Equation (2.10) may easily be derived by writing

$$|\psi_j^{(n+1)}\rangle = (1-\lambda h^{(n+\frac{1}{2})})|\psi_j^{(n)}\rangle + \lambda(\alpha_j|\psi_j^{(n)}\rangle + \sum_{k=1}^{j-1} \beta_{kj}|\psi_k^{(n)}\rangle),$$

and determining the values of α_j and the β_{kj} by requiring that

$$\langle\psi_j^{(n+1)}|\psi_k^{(n+1)}\rangle = \delta_{jk}.$$

12. In principle, Eq. (2.16) requires only that $[h,\rho] = \eta(1-\rho)$. However, the idempotency of ρ may then be invoked to show that η must be equal to zero.

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15. J. Cugnon, H. Doubre and H. Flocard, Nucl. Phys. in press; J. Cugnon, H. Doubre and H. Flocard, to be published.

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17. The imaginary time step method may also be used to obtain the unoccupied states. Indeed in the sum we have included the 10 lowest unoccupied states as well as all of the occupied states.

18. P. H. Heenen, P. Bonche and H. Flocard, in Proceedings of the meeting on Time dependent Hartree-Fock Orsay-Saclay, May 1979.

FIGURE CAPTIONS

Fig. 1.   The difference between the nth approximation to the HF energy

and the HF energy is plotted as a function of $t^{(n)} = n\Delta t$, for

several values of $\Delta t = \lambda\hbar$.

Fig. 2.   The difference between the nth approximation to the HF energy

and the HF energy is plotted as a function of $t^{(n)} = n\Delta t$, for

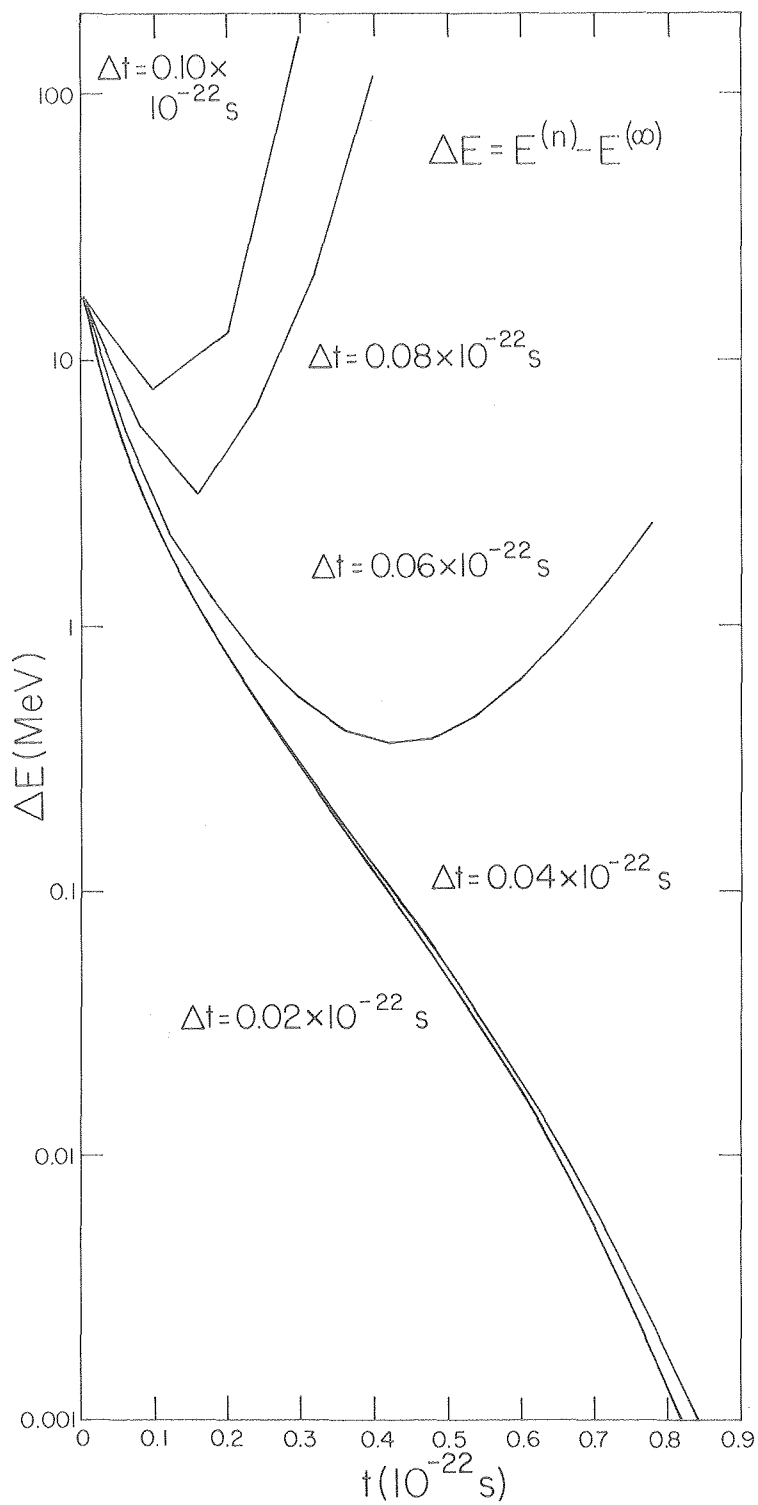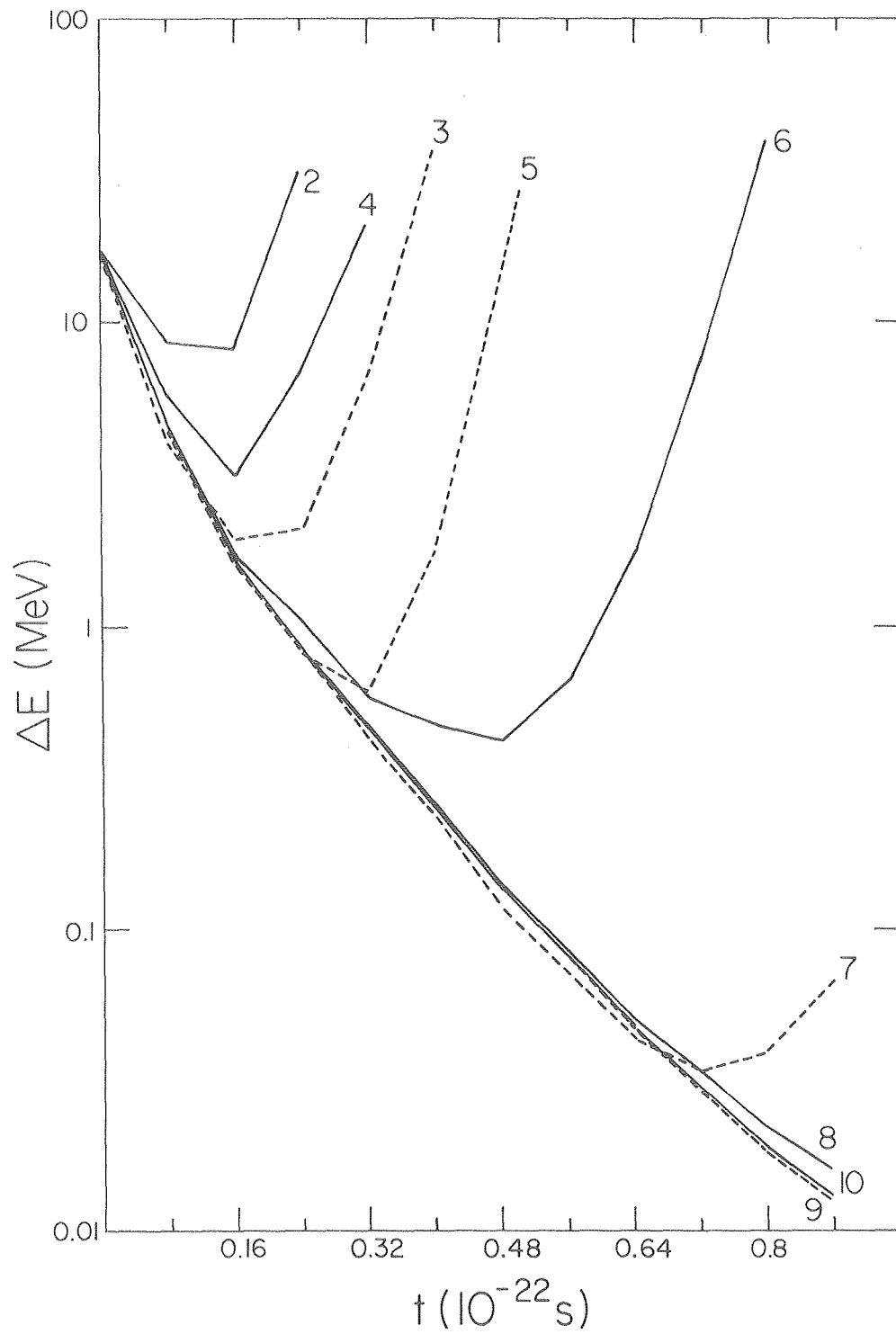expansions of the exponential operator consisting of from 2

to 10 terms.

$\Delta t = 0.10 \times 10^{-22} s$

$\Delta E = E^{(n)} - E^{(\infty)}$

$\Delta t = 0.08 \times 10^{-22} s$

$\Delta t = 0.06 \times 10^{-22} s$

$\Delta t = 0.04 \times 10^{-22} s$

$\Delta t = 0.02 \times 10^{-22} s$

$\Delta E (MeV)$

$t(10^{-22} s)$

Fig. 1

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Fig. 2

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